

This is a contributed topic entry on [computer simulations](#) and automata theory applications.

## 0.1 Computer simulations and automata theory applications in life sciences, theoretical biophysics, medicine and mathematical medicine

The applications of [computers](#) to biological and biomedical problem solving go back to the very beginnings of computer science, [automata theory](#), and mathematical biology. With the advent of more versatile and powerful computers, biological and biomedical applications of computers have proliferated so rapidly that it would be virtually impossible to compile a comprehensive review of all developments in this [field](#). Limitations of computer simulations in biology have also come under close scrutiny, and claims have been made that biological [systems](#) have limited information processing [power](#) [3]. Such general conjectures do not, however, deter biologists and biomedical researchers from developing new computer applications in biology and medicine. Microprocessors are being widely employed in biological laboratories both for automatic data acquisition/processing and modeling; one particular area, which is of great biomedical interest, involves fast digital image processing and is already established for routine clinical examinations in radiological and [Nuclear Medicine](#) centers. Powerful techniques for biological research are routinely employing dedicated, on-line microprocessors or array processors; among such techniques are: Fourier-transform [nuclear magnetic resonance \(NMR\)](#), [NMR](#) imaging (or [tomography](#)), [X-ray](#) tomography, [X-ray diffraction](#), high performance liquid chromatography, differential scanning calorimetry and [mass](#) spectrometry. Networking of laboratory microprocessors linked to a central, large memory computer is the next logical step in laboratory automation. Previously unapproachable problems, such as [molecular dynamics](#) of solutions, many-body interaction calculations and [statistical mechanics](#) of biological processes are all likely to benefit from the increasing access to the new generation of "[supercomputers](#)". In view of the large number, diversity and [complexity](#) of computer applications in biology and medicine, we could not review in any degree of detail all computer applications in these fields; instead, we shall be selective and focus our discussion on suggestive computer models of biological systems and those fundamental aspects of computer applications that are likely to continue to make an impact on biological and biomedical research. Thus, we shall consider unifying trends in mathematics, mathematical logics and computer science that are relevant to computer modeling of biological and biomedical systems. The latter are pitched at a more formal, abstract level than the applications and, therefore, encompass a number of [concepts](#) drawn from the abstract theory of sets and [relations](#), network theory, automata theory, Boolean and n-valued logics, [abstract algebra](#), topology and [category theory](#). The present analysis of [Relational Theories](#) in biology and computer simulation has also inspired a number of new results which are presented here as "Conjectures" since their proofs are too lengthy and too technical to be included in this review. In order to maintain a self-contained presentation-the definitions of the main concepts are given, with the exception of a minimum of simple mathematical concepts. The purpose of these theoretical [sections](#) is to provide the basis for approaching a number of basic biological questions:

- (1) What are the essential characteristics of a biological organism as opposed to an [automaton](#)?
- (2) Are biological systems recursively computable?
- (3) What is the structure of the simplest (primordial) organism?
- (4) What are the basic structures of neural and [genetic networks](#)?
- (5) What are the common properties of classes of biological organisms?
- (6) Which system [representations](#) are adequate for biodynamics?
- (7) What is the optimal strategy for modifying an organism through genetic engineering?
- (8) What is the optimal simulation of a biological system with a digital or analog computer?
- (9) What is life?